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WE CLAIM:

- 1. A crystal of IMPDH (ionisine monophosphate dehydrogenase) isolated from a bacterial preparation.
- 2. The crystal of claim 1 further characterized by ability to provide x-ray diffraction patterns useful to define molecular structures for bacterial IMPDH enzymes.
- 3. The crystal of claim 1 wherein the bacterial preparation is a pure culture of *Streptococcus pyogenes*.
- 4. A method for developing lead compounds for an inhibitor of bacterial IMPDH (inosine monophosphate dehydrogenase), said method comprising
 - a. obtaining\(a \) crystal of bacterial IMPDH;
 - b. recording x-ray diffraction data from said crystal;
 - c. using said diffraction data to generate an electron density map consistent with the model for the molecular structure of IMPDH; and
 - d. developing lead compounds for an inhibitor of bacterial IMPDH based on the map of three dimensional structural information of the molecular structure of IMPDN.
- 5. A crystalline molecule or molecular complex comprising an IMPDH binding pocket defined by the structural coordinates of IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455 according to Table 7 or a homologue of said molecule or molecular complex.
- 6. A crystalline molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids, according to Table 7, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has an amino acid sequence identity of 60% or greater relative to the *S. pyogenes* IMPDH binding pocket.
- 7. A crystalline IMPDH molecule comprising coordinates from *S. pyogenes* IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455.
- 8. A crystalline IMPDH molecule having (inosine monophosphate) IMP in its binding pocket.

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9. A computer generated representation of a molecule or molecular complex comprising a binding pocket defined by the following structural coordinates of *S. pyogenes* IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455.